

Supporting Information

Three Unprecedented Polycationic Templated Cupreous Thiocyanate Networks: Synthesis, Structure, and Properties

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Table S1. Bond Lengths (Å) and Angles (deg) for **1-3**

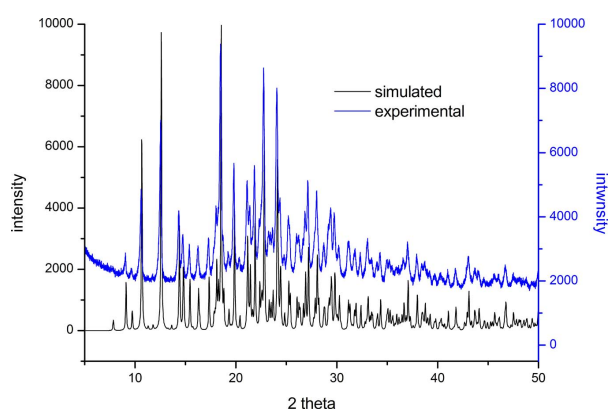
Compound 1					
Cu1- S1	2.3648(14)	Cu1- S3	2.3602(13)	Cu1- N1 ¹	2.023(4)
Cu1- N2	1.953(4)	Cu2- S2 ²	2.5188(16)	Cu2- N3	1.957(4)
Cu2- N4	1.983(4)	Cu2- N6 ³	2.021(4)	Cu3- S4	2.3432(14)
Cu3- S5	2.3633(16)	Cu3- S6	2.4018(14)	Cu3- N5 ⁴	1.954(4)
S2- Cu2 ⁵	2.5188(16)	N1- Cu1 ⁶	2.022(4)	N5- Cu3 ⁷	1.954(4)
N6- Cu2 ⁸	2.021(4)				
S3-Cu1- S1	111.97(5)	N1 ¹ -Cu1-S1	98.04(12)	N1 ¹ -Cu1- S3	111.23(13)
N2-Cu1-S1	112.48(14)	N2-Cu1- S3	109.45(12)	N2-Cu1-N1 ¹	113.34(17)
N3-Cu2-S2 ²	112.18(14)	N3-Cu2- N4	122.41(19)	N3-Cu2-N6 ³	113.48(18)
N4-Cu2-S2 ²	96.41(14)	N4-Cu2-N6 ³	110.39(18)	N6 ³ -Cu2-S2 ²	97.87(14)
S4- Cu3- S5	106.16(6)	S4- Cu3- S6	110.07(5)	S5- Cu3- S6	104.35(6)
N5 ⁴ -Cu3-S4	110.07(14)	N5 ⁴ -Cu3-S5	117.08(14)	N5 ⁴ -Cu3- S6	108.87(13)
C1-S1- Cu1	106.47(16)	C2-S2- Cu2 ⁵	111.22(17)	C3- S3- Cu1	103.75(15)
C4-S4- Cu3	109.88(16)	C5- S5- Cu3	104.63(17)	C6- S6- Cu3	110.44(15)
C1-N1-Cu1 ⁶	167.3(4)	C2-N2- Cu1	172.4(4)	C3-N3- Cu2	173.4(4)
C4-N4- Cu2	172.5(4)	C5-N5-Cu3 ⁷	173.5(4)	C6-N6-Cu2 ⁸	158.4(4)
Compound 2					
Cu1- S2	2.4091(12)	Cu1- S3	2.3518(12)	Cu1- N1	1.962(4)
Cu1- N2 ¹	2.013(3)	Cu2- S5	2.4275(12)	Cu2- N3	1.976(3)
Cu2- N4	1.971(4)	Cu2- N5 ²	1.998(3)	N2- Cu1 ³	2.013(3)
N5- Cu2 ⁴	1.998(3)				
S3-Cu1-S2	102.84(4)	N1-Cu1-S2	110.61(12)	N1-Cu1-S3	119.60(11)

[†] Electronic supplementary information (ESI) available: experimental and simulated powder XRD patterns, IR spectra, and the detailed crystallographic data and structural refinement parameters for **1-3**. CCDC reference numbers 900604 for **1**, 926422 for **2**, 926179 for **3**.

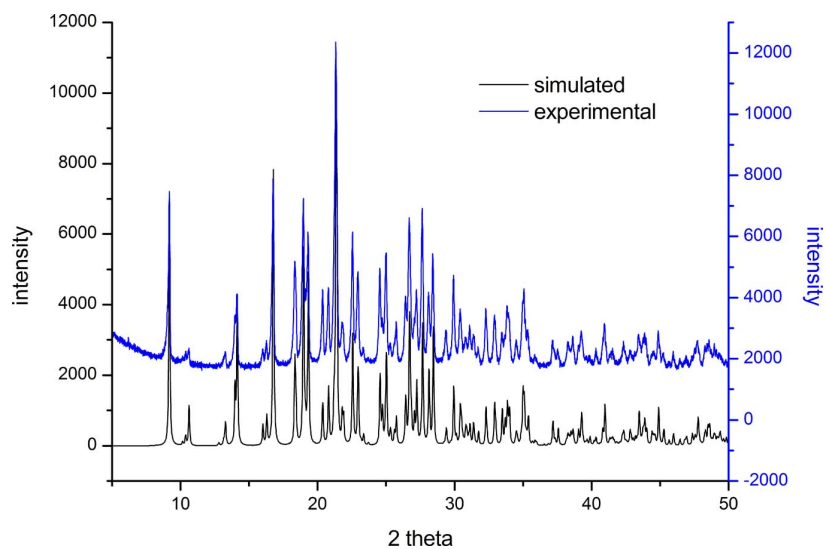
N1-Cu1-N2 ¹	108.47(14)	N2 ¹ -Cu1-S2	109.28(10)	N2 ¹ -Cu1-S3	105.59(12)
N3-Cu2- S5	101.66(11)	N3-Cu2- N5 ²	113.27(16)	N4-Cu2- S5	107.72(11)
N4-Cu2- N3	114.36(15)	N4-Cu2- N5 ²	109.33(13)	N5 ² -Cu2- S5	110.10(9)
C2- S2- Cu1	103.87(13)	C3-S3- Cu1	105.85(15)	C5-S5- Cu2	107.85(12)
C1-N1- Cu1	163.5(3)	C2-N2-Cu1 ³	162.7(3)	C3-N3-Cu2	166.4(4)
C4-N4-Cu2	166.6(3)	C5-N5- Cu2 ⁴	167.7(3)		
Compound 3					
Cu(1)-N(6)	1.975(6)	Cu(1)-N(1)	1.986(7)	Cu(1)-S(6)	2.377(2)
Cu(1)-S(1)	2.414(2)	Cu(2)-N(3)	1.957(7)	Cu(2)-N(2)	1.961(7)
Cu(2)-S(2)#1	2.334(2)	Cu(2)-S(3)	2.484(3)	S(2)-Cu(2)#4	2.334(2)
N(6)-Cu(1)-N(1)	110.7(3)	N(6)-Cu(1)-S(6)	107.9(2)	N(1)-Cu(1)-S(6)	114.86(18)
N(6)-Cu(1)-S(1)	115.7(2)	N(1)-Cu(1)-S(1)	106.56(19)	S(6)-Cu(1)-S(1)	100.96(7)
N(3)-Cu(2)-N(2)	121.2(3)	N(3)-Cu(2)-S(2)#1	115.3(2)	N(2)-Cu(2)-S(2)#1	109.0(2)
N(3)-Cu(2)-S(3)	110.5(2)	N(2)-Cu(2)-S(3)	99.8(2)	S(2)#1-Cu(2)-S(3)	97.19(9)
C(2)-N(1)-Cu(1)	173.6(6)	C(1)-N(2)-Cu(2)	160.3(7)	C(4)#2-N(3)-Cu(2)	158.7(7)
C(3)#3-N(6)-Cu(1)	166.7(7)	C(1)-S(1)-Cu(1)	100.6(3)	C(2)-S(2)-Cu(2)#4	101.3(3)
C(4)-S(3)-Cu(2)	123.7(3)	C(3)-S(6)-Cu(1)	104.8(3)		

^aSymmetry codes for **1**: ¹1-X,-1/2+Y,1/2-Z; ²-1+X,+Y,+Z; ³+X,1+Y,+Z; ⁴1/2+X,1/2-Y,1-Z; ⁵1+X,+Y,+Z; ⁶1-X,1/2+Y,1/2-Z; ⁷-1/2+X,1/2-Y,1-Z; ⁸+X,-1+Y,+Z. Symmetry codes for **2**: ¹-X,-1/2+Y,1-Z; ²-X,-1/2+Y,-Z; ³-X,1/2+Y,1-Z; ⁴-X,1/2+Y,-Z. Symmetry codes for **3**: #1 -x+1/2,y-1/2,z; #2 x+1/2,-y+3/2,-z; #3 x-1/2,y,-z+1/2; #4 -x+1/2,y+1/2,z; #5 x+1/2,y,-z+1/2; #6 x-1/2,-y+3/2,-z; #7 -x+1,-y+1,-z+1.

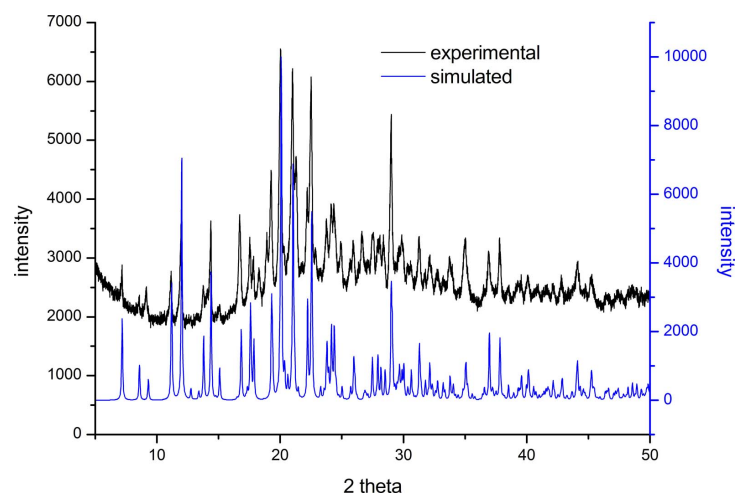
Fig. S1



(a) The PXRD pattern of compound **1**

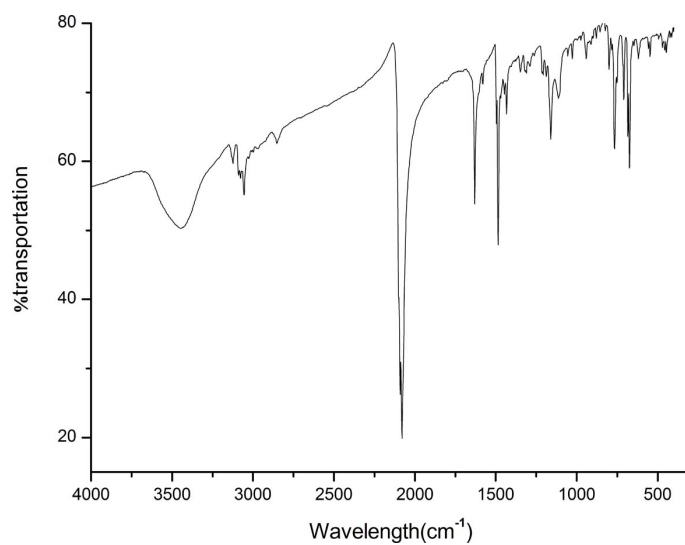


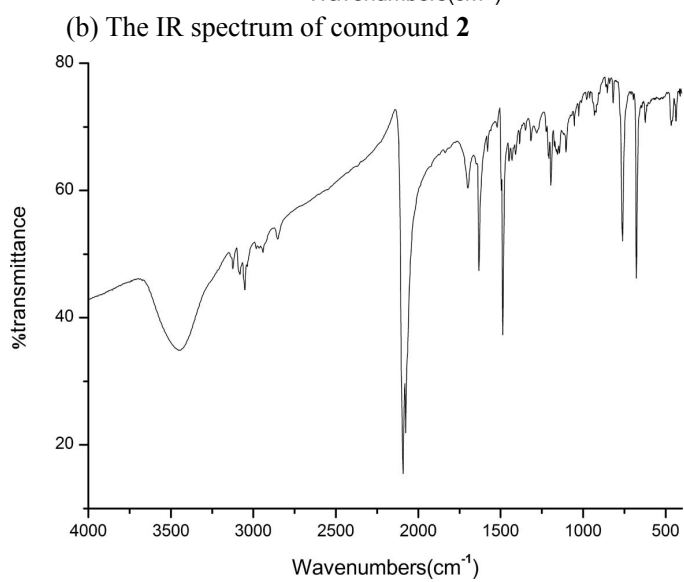
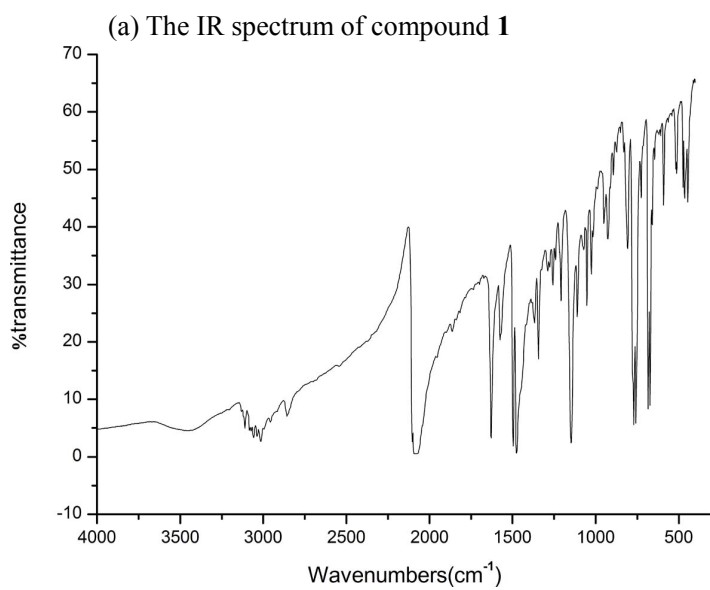
(b) The PXR D pattern of compound 2



(c) The PXR D pattern of compound 3

Fig. S2





(c) The IR spectrum of compound **3**